

Long and short time quantum dynamics: II. Kinetic regime

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Available online 18 July 2005

Abstract

Non-equilibrium Green's functions reduce to quantum kinetic equations in the kinetic regime, that is, if the quasi-classical, quasi-particle picture is valid. The classical tool yielding the kinetic equations, the Kadanoff–Baym Ansatz, has been improved and generalized to a whole Ansatz family including the so-called extended quasi-particle approximation. Each Ansatz produces a quantum kinetic theory: a quasi-particle kinetic equation and a functional of the quasi-particle distribution returning the average values of observables. In the extended quasi-particle model, the theory is physically consistent: causal, gauge invariant and conserving. This model leads to kinetic equations for dense Fermi liquids which combine the Landau quasi-particle drift with non-local scattering integrals in the spirit of the Enskog equation.

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PACS: 05.30.-d; 05.20.Dd; 05.60.Gg; 72.10.Bg; 72.20.Dp

Keywords: Non-equilibrium; Green functions; Quantum transport equations; Quasi-particles

1. Introduction

This second article of the series ([1], hereafter called Paper I, [2], hereafter called Paper III) will deal with quantum kinetic equations for quasi-particle distribution.

A prototype of all kinetic equations discussed in this article is the Boltzmann equation (for details see Paper I and reference therein)

$$\frac{\partial f}{\partial t} - \text{drift}[f(t)] = I_{\text{in}}[f(t)] - I_{\text{out}}[f(t)], \quad (1)$$

where the drift term is

$$\text{drift}[f(t)] = \frac{\partial \varepsilon}{\partial k} \frac{\partial f}{\partial r} - \frac{\partial \varepsilon}{\partial r} \frac{\partial f}{\partial k}. \quad (2)$$

This is an equation for a single-particle distribution function $f(k, r, t)$ in phase-space, representing a balance between the drift of particles (with energy $\varepsilon = \varepsilon_k + U(r, t)$ and velocity $\frac{\partial \varepsilon}{\partial k} = \frac{\partial \varepsilon_k}{\partial k}$ in the external force field $-\frac{\partial \varepsilon}{\partial r} = -\frac{\partial U}{\partial r}$), as given by the left-hand side of the BE, and the irreversible evolution due to collisions described by the scattering integrals I_{in} and I_{out} on the right-hand side. These integrals are local in space and time.

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From the time of Boltzmann, the kinetic theory developed in several streams. The following two will be the most important for this article. Within the classical kinetic theory, Enskog started the stream of investigations treating the non-localities of scattering events needed to describe dense gases [3–5]. By this step, virial corrections to the equation of state were included into the kinetic theory for the first time. The second main stream derived from the Boltzmann kinetic theory dealt with its quantum generalization. The first intuitive generalization of the Boltzmann equation for quantum systems was suggested by Nordheim [6] and Uehling and Uhlenbeck [7]. Later on, many versions of the quantum Boltzmann equation have been obtained by various methods of statistical physics [8–22]. In general, quantum generalizations of the Boltzmann equation placed emphasis on the quasi-particle description of the drift of particles and derivation of convenient local scattering integrals for various mechanisms of scattering. The classical kinetic theory concentrated on the problem of virial corrections in terms of properly treated non-local scattering integrals.

Here, we will demonstrate how the structure of the quantum Boltzmann equation emerges as a consistent quasi-classical approximation of the general transport equation for the Non-equilibrium Green functions (NGF). Second, we will show that within NGF, we can derive the kinetic equation, which has the same drift part as the quasi-particle Boltzmann equation of Landau type and, at the same time, it has scattering integrals, covering virial corrections, which are non-local in space and time.

We will follow the line of incorporating the quantum dynamical features increasingly, while retaining the formal framework of the quasi-classical limit of the NGF transport theory. First, we will discuss the emergence of quantum dynamics within the original Kadanoff–Baym approach to the NGF based on the Landau quasi-particle picture in Section 2. After discussion of the shortcomings of this approach in Section 3 we introduce an extended quasi-particle approximation (EQA) in Section 4. The EQA allows to introduce more subtle quantum effects into the quantum Boltzmann equation. A natural con-

struction of the quantum kinetic theory, consisting of two parts, will appear: we will construct a Quantum Kinetic Equation (QKE) for the quasi-particle distribution function and simultaneously a non-trivial functional between this distribution function and the single-particle density matrix describing real observables. The EQA also provides a possibility to create a kinetic theory for dense Fermi systems: in other words we can (within quasi-classical approximation of NGF transport theory) even derive a quantum kinetic equation which consistently describe quasi-particle and virial corrections at the same time. In Section 5 we will first show the essential constituents of the construction of such a non-local kinetic theory in the example of electron transport in semiconductors with resonant impurity levels. In this case, scattering integrals are non-local in time, but local in space. Finally, we will briefly discuss the more complicated case of a kinetic theory for dense Fermi liquid where full binary collisions are taken into account and scattering integrals of a relevant kinetic equation emerge as non-local both, in space and time.

2. NGF and quantum kinetic equations

The starting point for the real-time NGF approach is the electron correlation function (Paper I, [21,22]),

$$\begin{aligned} g^<(1, 2) &= \text{TR}(\hat{\rho}\psi^\dagger(2)\psi(1)) \\ &\equiv \langle\langle \psi^\dagger(2)\psi(1) \rangle\rangle, \end{aligned} \quad (3)$$

where, instead of x, t we introduce cumulative variables denoted by numbers, $1 \equiv x_1, t_1$. Here $\hat{\rho}$ is the full many-body statistical operator (typically, a grand canonical density matrix) and ψ^\dagger and ψ are field operators for particles (electrons throughout this article), all in the Heisenberg picture.

The single-electron reduced density matrix is then the time-diagonal element of this correlation function

$$\rho(x_1, x_2, t) = g^<(1, 2)|_{t_1, 2=t} \quad (4)$$

from which we can evaluate single-particle observables.

A complete set of correlation functions is obtained by introducing a complementary function, the correlation function for holes

$$g^>(1, 2) = \langle\langle \psi(1)\psi^\dagger(2) \rangle\rangle. \quad (5)$$

For these two functions $g^<$, $g^>$, Kadanoff and Baym developed a closed set of coupled dynamic equations, the KB formalism [8]. Here, we will use an equivalent, the Langreth–Wilkins set of equations ([23,24], Paper I) which, in addition, work with retarded (G^R) and advanced (G^A) Greens functions:

$$G^R(1, 2) = -i\theta(t_1 - t_2)(g^>(1, 2) + g^<(1, 2)), \quad (6)$$

$$G^A(1, 2) = i\theta(t_2 - t_1)(g^>(1, 2) + g^<(1, 2)). \quad (7)$$

2.1. Transport equation for correlation function

The starting point for the derivation of all kinetic equations in this article is the integral Dyson–Keldysh equation for the correlation function $g^<$, (Paper I and references therein):

$$g^< = G^R \sigma^< G^A. \quad (8)$$

This equation, with all integrations explicitly shown, reads

$$G^<(1, 2) = \int_{-\infty}^{t_1} d3 \int_{-\infty}^{t_2} d4 G^R(1, 3) \Sigma^<(3, 4) G^A(4, 2). \quad (9)$$

In this article we will deal only with the long-time (kinetic) regime, so initial conditions do not appear explicitly, as $t_0 = -\infty$; for details, see Paper I.

Since kinetic equations are, in principle, integro-differential equations, the first step toward kinetic equations from NGF will be to turn the Dyson–Keldysh equation into its integro-differential form:

$$-i(G_0^{-1} g^< - g^< G_0^{-1}) = i(G^R \sigma^< - \sigma^< G^A) - i(\Sigma^R g^< - g^< \Sigma^A). \quad (10)$$

This equation is the precursor of all quantum kinetic equations discussed in this article. Here, the Dyson equations

$$\{G^{R,A}\}^{-1} = G_0^{-1} - \Sigma^{R,A} \quad (11)$$

serve, in fact, as defining identities for the respective self-energies if we specify the free

Green's functions $G_0^{R,A}$. We define their inverse as incorporating the external field and the mean-field contributions to the potential energy in U_{eff} by the formula:

$$G_0^{-1}(1, 2) = \delta(1 - 2) \left(i \frac{\partial}{\partial t_2} - \epsilon \left(\frac{1}{i} \nabla_2 \right) - U_{\text{eff}}(x_2, t_2) \right). \quad (12)$$

The self-energy Σ is thus cleared of the mean field, that is, of a “singular” time-local component, by this definition.

To arrive at a quantum generalization of the Boltzmann equation, it is natural to convert the transport equation (10) for correlation function $g^<$ into a form which explicitly contains spectral properties of the system and has a shape which is more suitable for quasi-classical approximation. To this end, we first introduce into (10) spectral functions A and Γ by separating the imaginary and real parts of retarded and advanced functions

$$A = i(G^R - G^A), \quad G = \frac{1}{2}(G^R + G^A), \quad (13)$$

$$\Gamma = i(\Sigma^R - \Sigma^A), \quad \Sigma = \frac{1}{2}(\Sigma^R + \Sigma^A). \quad (14)$$

In the second step with the help of the following identities:

$$i(G^R \sigma^< - \sigma^< G^A) = i[G, \sigma^<]_- + \frac{1}{2}[A, \sigma^<]_+, \quad (15)$$

$$i(\Sigma^R g^< - g^< \Sigma^A) = i[\Sigma, g^<]_- + \frac{1}{2}[\Gamma, g^<]_+, \quad (16)$$

where $[A, B]_{\pm} = AB \pm BA$ are anticommutators or commutators, we rearrange (10) into the following equation:

$$-i[G_0^{-1} - \Sigma, g^<]_- - i[G, \sigma^<]_- = \frac{1}{2}[A, \sigma^<]_+ - \frac{1}{2}[\Gamma, g^<]_+. \quad (17)$$

This equation is often called the Generalized Kadanoff–Baym (GKB) Equation.

2.2. Kinetic equation for quasi-particle distribution function: Kadanoff–Baym approach

Our aim is to find a quantum generalization of the BE, in a controlled way, i.e., we want to find a kinetic equation for a distribution function $f(k, r, t)$ from the GKB equation as an asymptotic equation. Naturally, the first step is to introduce

the Wigner representation of the correlation function

$$g^<(\omega, k, r, t) = \int dx d\tau e^{i\omega\tau - ikx} \times g^<\left(r + \frac{x}{2}, t + \frac{\tau}{2}, r - \frac{x}{2}, t - \frac{\tau}{2}\right), \quad (18)$$

where $(r + \frac{x}{2}, t + \frac{\tau}{2}) \equiv 1$ and $(r - \frac{x}{2}, t - \frac{\tau}{2}) \equiv 2$ in the cumulative variable notation. From now on, we will use Roman types for operators in the cumulative variable representation and Sans-serif types for operators in Wigner's representation.

The expression for Wigner's distribution function

$$\rho(k, r, t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g^<(\omega, k, r, t), \quad (19)$$

has the essential property that it includes contributions from all independent energies ω . Thus, a perturbation scheme constructed for $g^<$ instead of ρ will enable us to retain the energy as an independent variable until we select how to determine the energy of a particle from its position in phase space. By this step, we will find a proper distribution function by avoiding the problems with the high momenta tails of Wigner's function (see Paper I). The existence of the independent energy permits to distinguish two very different contributions in the transport equations for the correlation function $g^<$. First is the on-shell contributions, for which a dispersion relation between the energy and the position of the particle in phase space holds. Second is the off-shell contributions, for which no such relation exists. As we will see later, the possibility of this distinction leads to a formulation of the perturbation schemes which better suit the demands of the kinetic equations. To summarize this philosophy, we will close the perturbative expansion for $g^<$. A quantum kinetic equation will be derived as an asymptotic limit of the equation for $g^<$. This asymptotic equation is not closed for the Wigner's distribution, but only for the on-shell part of $g^<$ which can be interpreted as the quasi-particle distribution. The observables will be obtained from $g^<$ in the second step via (19).

2.2.1. Quasi-classical approximation

To proceed towards obtaining a kinetic equation, we now need to convert the GKB Equation (17) into the Wigner representation. For matrix products, $C = AB$, it reads

$$c = \exp\left(\frac{i}{2} \left(\frac{\partial}{\partial\omega} \frac{\partial}{\partial t'} - \frac{\partial}{\partial t} \frac{\partial}{\partial\omega'} - \frac{\partial}{\partial k} \frac{\partial}{\partial r'} + \frac{\partial}{\partial r} \frac{\partial}{\partial k'} \right)\right) \times a(\omega, k, r, t) b(\omega', k', r', t')_{\omega'=\omega, k'=k, r'=r, t'=t}. \quad (20)$$

The Boltzmann equation is known to be valid only for slowly varying fields. For this case we can expect that a dependence on the hydrodynamical variables r and t will be proportional to gradients of the external fields, i.e., small. In this situation, the gradient expansion (20) can be approximated by its lowest order terms. The anticommutator is also in gradients; thus, it is approximated by a simple product, $C = \frac{1}{2}[A, B]_+$,

$$c = ab. \quad (21)$$

The commutator is odd in gradients and it thus turns to the Poisson bracket, $C = -i[A, B]_-$,

$$c = [a, b] \equiv \frac{\partial a}{\partial\omega} \frac{\partial b}{\partial t} - \frac{\partial a}{\partial t} \frac{\partial b}{\partial\omega} - \frac{\partial a}{\partial k} \frac{\partial b}{\partial r} + \frac{\partial a}{\partial r} \frac{\partial b}{\partial k}. \quad (22)$$

Using Eqs. (21) and (22) we find the GKB Equation (17) in the gradient approximation

$$[\omega - \epsilon - U_{\text{eff}} - \sigma, g^<] + [g, \sigma^<] = a\sigma^< - \gamma g^<. \quad (23)$$

This equation is a good starting point for quantum generalizations of the BE.

2.2.2. Kadanoff–Baym ansatz

Contrary to the KB equation, which is the equation for $g^<(\omega, k, r, t)$, any kinetic equation of the Boltzmann type is an equation for a distribution function $f(k, r, t)$, so that there is no independent energy variable in it. Therefore, any construction of an asymptotic kinetic equation from the KB equations is a means to find an auxiliary functional $g^<[f]$ by which the independent energy becomes fixed and related to the phase-space variables. As a starting point for their construction of the auxiliary functional Kadanoff and Baym suggested the relation

$$g^<(\omega, k, r, t) \approx \phi(\omega, k, r, t) a(\omega, k, r, t), \quad (24)$$

i.e. they assumed that the relation between the correlation function $g^<$, the spectral function a and the Fermi–Dirac distribution f_{FD} , which is exact in equilibrium, was approximately valid close to equilibrium also for a non-equilibrium function ϕ . In the following step they eliminated the energy argument from ϕ by the assumption that the scattering rate was small, so that the spectral function had a singularity

$$a(\omega, k, r, t) \approx 2\pi\delta(\omega - \epsilon - U_{\text{eff}}(r, t)). \quad (25)$$

The energy argument of ϕ can be replaced by the mean-field energy $\epsilon + U_{\text{eff}}$. Kadanoff and Baym proposed to approximate $g^<$ as [8]

$$g^<(\omega, k, r, t) \approx f(k, r, t)a(\omega, k, r, t) \quad (26)$$

$$\approx f(k, r, t)2\pi\delta(\omega - \epsilon - U_{\text{eff}}(r, t)). \quad (27)$$

Taking approximation (26), one does not obtain the BE, since this approximation leads to the violation of energy conservation of individual scattering events. Kadanoff and Baym thus used the (mean-field) non-renormalized pole approximation (27), which is called the Kadanoff and Baym Ansatz (KBA).

2.2.3. BE in the mean-field approximation

From the KB equation (23) and the KB Ansatz (27) of $g^<$ we obtain

$$2\pi\delta(\omega - \epsilon - U_{\text{eff}})[\omega - \epsilon - U_{\text{eff}} - \sigma, f] + [g, \sigma^<] = 2\pi\delta(\omega - \epsilon - U_{\text{eff}})(\sigma^< - \gamma f), \quad (28)$$

where we used $[\omega - \epsilon - U_{\text{eff}}, \delta(\omega - \epsilon - U_{\text{eff}})] = 0$, and the δ -function can be extracted from the first Poisson bracket.

At this point, Kadanoff and Baym adopted an idea that only the pole terms, in other words, only the terms with the δ -function contributed to the BE. They completely neglected the Poisson bracket $[g, \sigma^<]$. By this step, Kadanoff and Baym eliminated the ω -dependence using the pole value, $\omega = \epsilon + U_{\text{eff}}$, and they derived the following kinetic equation:

$$\frac{\partial f}{\partial t} + \frac{\partial \epsilon}{\partial k} \frac{\partial f}{\partial r} - \frac{\partial U_{\text{eff}}}{\partial r} \frac{\partial f}{\partial k} = I_{\text{in}}[f] - I_{\text{out}}[f], \quad (29)$$

where the scattering integrals are given by

$$I_{\text{in}}[f] = \sigma_{\omega=\epsilon+U_{\text{eff}}}^<, \quad (30)$$

$$I_{\text{out}}[f] = f\gamma_{\omega=\epsilon+U_{\text{eff}}}. \quad (31)$$

2.2.4. BE in the quasi-particle approximation

To recover a quasi-particle BE for metals, Prange and Kadanoff [25] modified the original KB Ansatz and used its renormalized version by taking the spectral function as

$$a(\omega, k, r, t) \approx 2\pi\delta(\omega - \epsilon - U_{\text{eff}}(r, t) - \sigma(\omega, k, r, t)) = z 2\pi\delta(\omega - \epsilon), \quad (32)$$

where z is the wave-function renormalization

$$z = \frac{1}{1 - \frac{\partial \sigma}{\partial \omega} |_{\omega=\epsilon}}. \quad (33)$$

Following the approach of Kadanoff and Baym, it is assumed that a major contribution to the spectral weight concentrates in the pole, i.e., $z \approx 1$, and off-pole contributions are negligible. The energy argument of ϕ can be, in this case, substituted by the quasi-particle energy ϵ

$$g^<(\omega, k, r, t) \approx f(k, r, t)z 2\pi\delta(\omega - \epsilon). \quad (34)$$

We will call also this auxiliary functional $g^<[f]$ the KB Ansatz, even if Kadanoff and Baym originally suggested its simpler, non-renormalized, version. For obvious reasons, the use of this modified functional for $g^<$ in the KB equation is known as the quasi-particle approximation (QA).

Combining the KB equation (23) and quasi-particle KBA (34) for $g^<$, we have

$$z 2\pi\delta(\omega - \epsilon)[\omega - \epsilon - U_{\text{eff}} - \sigma, f] + [g, \sigma^<] = z 2\pi\delta(\omega - \epsilon)(\sigma^< - \gamma f), \quad (35)$$

where we used $[\omega - \epsilon - U_{\text{eff}} - \sigma, \delta(\omega - \epsilon - U_{\text{eff}} - \sigma)] = 0$. The δ -function can then be extracted from the first Poisson bracket.

To proceed further, following Kadanoff and Baym, first, the Poisson bracket $[g, \sigma^<]$ is neglected. We will discuss the meaning of this neglect later. Second, in the two terms proportional to the δ -function the ω -dependence is eliminated using the pole value, $\omega = \epsilon$. The terms with the δ -function contribute to the BE. The gradient

term reads

$$z 2\pi\delta(\omega - \varepsilon)[\omega - \varepsilon - U_{\text{eff}} - \sigma, f] \\ = 2\pi\delta(\omega - \varepsilon)\left(\frac{\partial f}{\partial t} + \frac{\partial \varepsilon}{\partial k} \frac{\partial f}{\partial r} - \frac{\partial \varepsilon}{\partial r} \frac{\partial f}{\partial k}\right), \quad (36)$$

where we have used $\partial_{k,r}(\varepsilon + U_{\text{eff}} + \sigma)_{\omega=\varepsilon} = z^{-1}\partial_{k,r}\varepsilon$. The wave function renormalization on the scattering integral side remains uncompensated; therefore, one finds

$$\frac{\partial f}{\partial t} + \frac{\partial \varepsilon}{\partial k} \frac{\partial f}{\partial r} - \frac{\partial \varepsilon}{\partial r} \frac{\partial f}{\partial k} = I_{\text{in}}[f] - I_{\text{out}}[f], \quad (37)$$

where the scattering integrals are given by

$$I_{\text{in}}[f] = z\sigma_{\omega=\varepsilon}^<, \quad (38)$$

$$I_{\text{out}}[f] = fz\gamma_{\omega=\varepsilon}. \quad (39)$$

This equation coincides with the BE for the quasi-particle distribution known from the theory of metals. Scattering integrals are functionals of the quasi-particle distribution, once the KB Ansatz (34) is also applied to the internal Green's functions $g^{>,<}$ of the self-energies $\sigma^{>,<}$ in the scattering integrals.

2.2.5. Observables

All single particle observables are determined by the single-particle density matrix ρ , whose dependence on the distribution function f is given by (19). According to (19), we obtain different expressions for observables in the mean-field and the quasi-particle approximation.

In the mean-field KBA (27)

$$\rho = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g^< = f, \quad (40)$$

so that we deal with the crudest approximation of the observables, which incorporates the quasi-particle features only through f .

In the quasi-particle KBA (34)

$$\rho = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g^< = zf, \quad (41)$$

the quasi-particle features additionally also appear in the renormalization function z . This approximation is, unfortunately, not consistent: in the simple quasi-particle approximation used, the off-shell part of the spectral function is missing. Correspondingly, this quasi-particle approxima-

tion does not fulfill the sum rule mandatory for any consistent spectral function

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} a = 1, \quad (42)$$

since

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} 2\pi z\delta(\omega - \varepsilon) = z. \quad (43)$$

In addition to the above-mentioned shortage, the quasi-particle approximation provides the oversimplified relation (41) between the density matrix ρ and quasi-particle distribution function f . As a result, the kinetic theory based on the plain quasi-particle approximation is not able to describe backflows known from the theory of metals as we can see from (41).

It is clear that the approximation of the spectral function only by its pole (“on-shell”) part and the corresponding quasi-particle approximation for $g^<$ is not sufficient for obtaining a consistent quasi-particle kinetic theory. We will show in the next section still further reasons for including the off-shell part of the spectral function into a consistent quantum kinetic theory.

3. Shortcomings of the KB approach

The first shortcoming of the Kadanoff and Baym approach has already been discussed: it does not use a spectral function for the construction of the quasi-particle theory, but it considers only its pole part. This neglect of the off-shell part of the spectral function goes hand in hand with the neglect of the off-shell term $[g, \sigma^<]$.

We will now discuss this second shortcoming of the KB approach. The reason for the neglect $[g, \sigma^<]$ within the Kadanoff and Baym approach is basically the fact that there is no clue as to how to handle $[g, \sigma^<]$ using the KBA. The cause of the difficulty emerges directly from its physical meaning. We can adopt as an illustration $G = \text{Re}G^{\text{R}}$ corresponding to the free particle propagator

$$g^{\text{R}}(\omega, k) = \frac{\wp}{\omega - \frac{k^2}{2m}} - i\pi\delta\left(\omega - \frac{k^2}{2m}\right). \quad (44)$$

According to the definitions of G , see Eq. (13), we can see that G is given by the first (principal value) term. It therefore describes the off-shell propagation with $\omega \neq \frac{k^2}{2m}$. In other words, the gradient term $[g, \sigma^<]$ corresponds to the off-shell drift of particles. Off-shell contributions are, however, not taken into account in the usual treatment of the Boltzmann equation. $g^<$ constructed from KB ansatz is non-zero only in the pole $\omega = \varepsilon$ and so there is no way in which to proceed using the KB Ansatz, other than to neglect $[g, \sigma^<]$. Correspondingly, neglecting this term we deal only with the pole part of the KB equation. Using only the pole approximation of the correlation function $g^<$ (KBA) we then naturally arrive at the kinetic theory which takes into account only the on-shell propagation of particles.

The question arises, whether there is a method of incorporating the off-shells into the quantum kinetic theory, and, at the same time, to overcome the inconsistencies of the Kadanoff and Baym approach. The essential step in this direction was taken by Botermans and Malfliet [26]. They recognized the off-shell character of the gradient (drift) term $[g, \sigma^<]$ and came to the conclusion that this term can be included in the derivation of the BE only if $g^<$ also includes the off-shell part. To our knowledge, they were the first to suggest (in Ref. [26]) an effective method on how to incorporate the off-shell part of $g^<$ into the asymptotic kinetic theory based on NGF: they showed that the off-shell drift $[g, \sigma^<]$ compensates the off-shell part of $[\omega - \epsilon - U_{\text{eff}} - \sigma, g^<]$.

In this article, we will not discuss the original Botermans and Malfliet approach, which is sometimes called Botermans and Malfliet substitution in the field of nuclear physics [27]. To show the essential steps taken toward obtaining included the kinetic theory with off shells contributions, we will follow an approach in the next section developed originally for deriving the quasi-particle BE for semiconductors in Refs. [28,29]. Before starting we will first discuss here the consequence of the neglect of the off-shell contribution $[g, \sigma^<]$ for the causality of the kinetic theory.

3.1. Causality and Kadanoff–Baym approach

We analyzed the neglect of $[g, \sigma^<]$ in the Wigner representation. For a further improvement of the quantum kinetic equations it is useful to consider this neglect in the representation-less, two-time structure of the exact GKB Equation. In other words, we will discuss the meaning of $[G, \sigma^<]$, which is the two-time precursor to the corresponding quasi-classical term $[g, \sigma^<]$.

The time structure of the term reads:

$$\begin{aligned} i[G, \sigma^<]_-(t_1, t_3) = & +\frac{i}{2} \int_{-\infty}^{t_1} d\bar{t} G^R(t_1, \bar{t}) \sigma^<(\bar{t}, t_3) \\ & +\frac{i}{2} \int_{t_1}^{\infty} d\bar{t} G^A(t_1, \bar{t}) \sigma^<(\bar{t}, t_3) \\ & -\frac{i}{2} \int_{t_3}^{\infty} d\bar{t} \sigma^<(t_1, \bar{t}) G^R(\bar{t}, t_3) \\ & -\frac{i}{2} \int_{-\infty}^{t_3} d\bar{t} \sigma^<(t_1, \bar{t}) G^A(\bar{t}, t_3). \end{aligned} \quad (45)$$

By extending the integrations the second and the third terms violate the causality: the rearrangements of the GKB Equation (8) leading to the KB equation (17) with commutators and anti-commutators disturb the strictly causal structure of individual terms of the original transport equation.

Without neglects in the KB equation (17), there is, however, no violation of causality in this equation since the causality is reestablished via the corresponding anti-commutator on the right-hand side of the KB equation:

$$\begin{aligned} \frac{1}{2} [A, \sigma^<]_+(t_1, t_3) = & \frac{i}{2} \int_{-\infty}^{t_1} d\bar{t} G^R(t_1, \bar{t}) \sigma^<(\bar{t}, t_3) \\ & -\frac{i}{2} \int_{t_1}^{\infty} d\bar{t} G^A(t_1, \bar{t}) \sigma^<(\bar{t}, t_3) \\ & +\frac{i}{2} \int_{t_3}^{\infty} d\bar{t} \sigma^<(t_1, \bar{t}) G^R(\bar{t}, t_3) \\ & -\frac{i}{2} \int_{-\infty}^{t_3} d\bar{t} \sigma^<(t_1, \bar{t}) G^A(\bar{t}, t_3). \end{aligned} \quad (46)$$

The second and the third terms again do not obey causality, but, at the same time, they precisely

compensate the causality violation by the anticausal terms of the commutator $[G, \sigma^<]_-$.

From the above, we can see, however, that causality of the theory is immediately lost, if $[G, \sigma^<]_-$ is neglected in the KB equation. In other words, the elementary Kadanoff and Baym approach deals incorrectly with the scattering-in, since only the anti-commutator part $\frac{1}{2}[A, \sigma^<]_+$ is retained, while the associated commutator $[G, \sigma^<]_-$ is neglected.

To retain a correct causal description, the commutator term $[G, \sigma^<]_-$ cannot be neglected, but it must be included in the drift part. As we have already seen, this term has an off-shell character in the Wigner representation. Correspondingly, it does not fit with the purely pole character of the Kadanoff–Baym Ansatz for the correlation function. This means that to include the off-shell term $[g, \sigma^<]$ in the approximation of the KB equation, we also have to include the off-shell term in the approximation for the correlation function $g^<$. At the same time, it is clear that the Boltzmann equation has the appearance of the on-shell (pole) propagation, i.e. it corresponds to the long-time approximant of the KB equation. The off-shell propagation, on the other hand, corresponds to the short time scale and so we cannot expect it to directly enter the BE equation.

4. Kinetic equations and extended quasi-particle approximation

We can solve the problem of the off-pole character of $[g, \sigma^<]$ and the pole character of the BE by taking advantage of the existence of two separate time scales, the short time scale and the long-time one, in any system, which can be described in the quasi-particle picture. The long space and time scale (also called hydrodynamic) is related to perturbations of a system while short (microscopic) scale deals with individual, local collisions of a particle (an electron). If the time and space characteristics of the perturbation as its frequency and length on which it changes substantially are much larger than corresponding characteristics of collisions (frequency of individual collisions, range of scattering potential), the

quasi-particle description works; see Paper I. It is also clear that the separation of scales is not related only to the quasi-particle picture, but it also indicates that the quasi-particle picture works well only in the quasi-classical limit. Supposing that a condensed system and its perturbations fulfill these scale separation conditions, we can consider the consequences for the movement of the electrons through the system and for the resulting kinetic theory. In a condensed system, such as a metal or a semiconductor, an individual electron undergoes, in the course of its travel, many short-range scattering events, and it polarizes its surrounding. This leads to a gradual change of the dispersion relation between its energy and momentum. This newly emerging dispersion relation corresponds to a new elementary excitation in a system, the electron-like quasi-particle instead of the original free electron having the bare dispersion relation. Accordingly, we can describe the diffusion of electrons, which includes large number of interactions on the long, hydrodynamical scale, as a diffusion of quasi-particles. This is the deeprooted physical reason as to why the distribution function of the Boltzmann equation describes quasi-particles. On the other hand, individual collisions and observables are related to the free propagation between the particle interactions.

4.1. Separation of two time scales

As a result, the quasi-particle kinetic theory has to be based on the separation of two time scales, long and short, and consequently it has to have two parts:

1. Quasi-particle kinetic equation (corresponding to long-time scale) which is a balance equation for diffusion and collisions of quasi-particles.

2. Auxiliary functional between quasi-particle distribution function and single-particle density matrix (corresponding to short time scale) which relates quasi-particles to bare particles.

Since quasi-particles work in the quasi-classical limit, we can view this separation either from the point of view of a more general time picture or within the energy picture in the Wigner representation. Correspondingly, we have a separation either of the long and short time scales, or,

equivalently, the pole and off-pole parts. We will follow the separation in the time picture.

4.1.1. Separation of on-shell and off-shell parts of the spectral function

This can be done by writing the spectral function as

$$A = S + B, \quad (47)$$

where

$$S = \frac{i}{2}(G^R \Gamma A - A \Gamma G^A) \quad (48)$$

consists mainly of the on-shell contribution, and

$$B = \frac{1}{2}(G^R \Gamma G^R + G^A \Gamma G^A) \quad (49)$$

includes mainly the off-shell part, as we can see from their evaluation in equilibrium, where the singular part reads

$$s = \frac{1}{2} \gamma a^2 = \frac{\frac{1}{2} \gamma^3}{((\omega - \epsilon - U_{\text{eff}} - \sigma)^2 + \frac{1}{4} \gamma^2)^2}. \quad (50)$$

In the limit $\gamma \rightarrow 0$, $s \rightarrow z 2\pi\delta(\omega - \epsilon)$.

The regular part

$$\begin{aligned} b &= \left(g^2 - \frac{1}{4} a^2 \right) \gamma \\ &= \frac{(\omega - \epsilon - U_{\text{eff}} - \sigma)^2 \gamma - \frac{1}{4} \gamma^3}{((\omega - \epsilon - U_{\text{eff}} - \sigma)^2 + \frac{1}{4} \gamma^2)^2} \end{aligned} \quad (51)$$

has a dominant contribution in the off-pole region. Integration over ω in a finite vicinity of the pole asymptotically approaches zero in the limit $\gamma \rightarrow 0$, since b changes its sign in the very vicinity of the pole.

4.1.2. Separation of the on-shell and off-shell parts of the correlation function

In correspondence with the separation of the on-shell and off-shell parts of the spectral function, we can separate the on-shell and off-shell parts of the correlation function $g^<$ (from the Dyson–Keldysh (8)) by writing it as a sum of the on-shell contribution $\lambda^<$ and the off-shell part $\xi^<$,

$$g^< = \lambda^< + \xi^<, \quad (52)$$

where the on-shell part

$$\lambda^< = \frac{i}{2}(G^R \sigma^< A - A \sigma^< G^A), \quad (53)$$

has the same structure as S and the off-shell part is reminiscent of B ,

$$\xi^< = \frac{1}{2}(G^R \sigma^< G^R + G^A \sigma^< G^A). \quad (54)$$

This is similar for $> \longleftrightarrow <$. Evidently, this separation directly parallels the separation of the spectral function.

Definitions (53) and (54) are, at the same time, equations of motion for correlation functions $\lambda^<$ and $\xi^<$. These two equations are equivalent to the GKB Equation for $g^<$. Eqs. (53) for $\lambda^<$ and (54) for $\xi^<$ are mutually coupled via the self-energy that depends on $g^{>,<}$, i.e. on $\lambda^{>,<} + \xi^{>,<}$.

Even if Eqs. (52)–(54) are equivalent to the GKB Equation (8), they provide a very different starting point for approximations which lead to kinetic equations, since within them, the off-shell and on-shell parts are separated in advance, before the construction of an asymptotic kinetic theory of the Boltzmann type. If the off-shell contributions are not separated in advance, they will be either lost (by a neglect of the off-shell drift $[g, \sigma^<]$) or mixed up with the on-shell contributions (by integration over the energy using e.g. the Ansatz with all spectral functions). In the former case, we would obtain a theory missing some off-shell processes; in the latter case, we would arrive at a theory with some unphysical off-shell contributions.

4.1.3. Fermi Golden rule and completed collision

We now show that the splitting of $g^<$ in pole and off-pole parts corresponds to the idea of the Fermi Golden rule, which is present in some form in any kinetic theory of the Boltzmann type.

Fermi's Golden rule is based on the identification of the on-shell contributions by integrating through the collision up to an infinite future. In this infinitely distant time, only the on-shell contributions survive, while the off-shell contributions die out by dephasing. This corresponds to the fact that, after any collision, a free asymptotic state is reached before the onset of the next collisional event. This procedure, sometimes called completed collision, also forms the basis of the original BE in the kinetic theory of gases.

We will just go through the same procedure within the NGF, i.e. for correlation function $g^<$.

To show how this procedure works, let us focus on the time-diagonal of the GKB Equation (8)

$$g^<(t, t) = \int_{-\infty}^t d\tilde{t} G^R(t, \tilde{t}) \int_{-\infty}^{\tilde{t}} d\tilde{\sigma}^<(\tilde{t}, \tilde{\sigma}) G^A(\tilde{\sigma}, t). \quad (55)$$

Following the idea of completed collision, we now extend the time integration over \tilde{t} in (55) to an infinite future using the spectral function A instead of the propagator G^R

$$\lambda_A^<(t, t) = -i \int_{-\infty}^{\infty} d\tilde{t} A(t, \tilde{t}) \int_{-\infty}^{\tilde{t}} d\tilde{\sigma}^<(\tilde{t}, \tilde{\sigma}) G^A(\tilde{\sigma}, t). \quad (56)$$

Accordingly, this integration into the future pushes out the off-shell contributions so that $\lambda_A^<$ is dominated by the on-shell ones.

Because of the GF symmetry, we can also introduce an adjoint correlation function replacing G^A by the spectral function A

$$\lambda_R^<(t, t) = i \int_{-\infty}^t d\tilde{t} G^R(t, \tilde{t}) \int_{-\infty}^{\tilde{t}} d\tilde{\sigma}^<(\tilde{t}, \tilde{\sigma}) A(\tilde{\sigma}, t). \quad (57)$$

The symmetric form, obtained as the average of λ_A and λ_R , gives just the on-shell part of $g^<$ as already introduced

$$\lambda^< = \frac{1}{2}\lambda_A^< + \frac{1}{2}\lambda_R^<. \quad (58)$$

From the fact that the idea of the completed collision is involved in the construction of λ , and, as a result, this function mainly has a pole character, it is clear that the equation of motion for λ is the starting point for the derivation of any asymptotic kinetic equation. At the same time, the procedure of the completed collisions in conflict with the principle of causality. The situation is different from the case considered in Section 3, where the $[g, \sigma^<]$ has been neglected. At present, the causality of the theory is preserved by the complementary equation for ξ .

4.2. Quasi-classical approximation

To obtain a proper kinetic equation of the Boltzmann type, and a corresponding method on, how to calculate observables, we have to deal with

Eqs. (54) and (53) differently, because of their different characters.

4.2.1. Quasi-classical equation for ξ

$\xi^<$ is associated with the off-pole correction. Since the off-pole terms correspond to the local (short time) scale, this function has to be treated directly within its integral form. In the quasi-classical limit, Eq. (54) reads

$$\xi^< = \frac{1}{2}(g_R^2 + g_A^2)\sigma^< = \left(g^2 - \frac{1}{4}a^2\right)\sigma^<. \quad (59)$$

4.2.2. Quasi-classical equation for λ

$\lambda^<$ is, on the other hand, associated with the pole dynamics. We therefore expect that, at the end, it turns into the quasi-particle Boltzmann equation. The BE is a differential equation; therefore, in analogy with the Kadanoff and Baym approach, we have to convert (53) into the differential form and only after this can we assign the quasi-classical limit.

After rather tedious algebraic manipulations, we obtain

$$[\omega - \epsilon - U_{\text{eff}} - \sigma, \lambda^<] - \frac{1}{2}[\gamma, ag\sigma^<] = \sigma^<s - \gamma\lambda^<. \quad (60)$$

This equation is a precursor of the quasi-particle BE.

4.3. Extended quasi-particle approximation

Now we wish to transform Eq. (60) into a kinetic equation. To this end, in analogy with the Kadanoff and Baym approach, we have to find an auxiliary functional $\lambda[f]$. We are bound, however, to find not only the auxiliary functional of the pole part $\lambda[f]$ but also its off-pole counterpart $\xi^<[f]$, since in (60) we have $\sigma^<[g^< = \lambda^< + \xi^<]$.

This completely follows our arguments that shortages of the Kadanoff and Baym approach are related to the fact that only the pole part of the spectral function a and the corresponding correlation function $g^<$ were taken into account in this approach.

To include both the pole and off-pole parts of spectral function a and correlation function $g^<$ in a consistent manner, we generalize the so-called

small γ expansion used in equilibrium, to non-equilibrium situations.

This approximation was, in equilibrium, introduced under several different names. For the first time it was, according to our knowledge, used by Craig in 1966 [30] and later on by Zimmerman [31] and Kremp and others [32] who called it the limit of small scattering rates. Schmidt and Röpke [33] worked with this approximation under the name of the generalized Beth–Uhlenbeck approach. Kohler and Malfliet [34] made a detailed comparison of this approximation with the quasi-particle approximation, calling it the extended quasi-particle approximation (EQA). The non-equilibrium version of this approximation was introduced in [28] and [29] as a generalization of the Kadanoff and Baym Ansatz which we will discuss here. In these articles, it was called the small γ expansion. Somewhat later, Bornath and others [35] used a similar approximation without any specific name.

Here, we will call the non-equilibrium version of the limit of small scattering rates, $\gamma \rightarrow 0$, the extended quasi-particle approximation (EQA).

4.3.1. Spectral functions in EQA

In the linear order in small γ , i.e. in the limit of small scattering rates $\gamma \rightarrow 0$, the spectral function s has a clear pole character and behaves as a δ function

$$s = 2\pi\delta(\omega - \epsilon_k - U_{\text{eff}} - \sigma) = 2\pi z\delta(\omega - \epsilon), \quad (61)$$

where ϵ is the quasi-particle energy given by

$$\epsilon(k, r, t) = \epsilon_k + U_{\text{eff}} + \sigma(\omega, k, r, t)|_{\omega=\epsilon(k, r, t)} \quad (62)$$

and z is the wave-function renormalization factor

$$z(k, r, t) = 1 + \frac{\partial \sigma(\omega, k, r, t)}{\partial \omega} \Big|_{\omega=\epsilon(k, r, t)}, \quad (63)$$

which is just the $\gamma \rightarrow 0$ limit of a more general formula (33).

Contrary to s , the spectral function b has, as expected, an off-shell character. In the $\gamma \rightarrow 0$ limit

$$b = \gamma \frac{\wp'}{\omega - \epsilon} = \text{Re} \frac{\gamma}{(\omega - \epsilon + i0)^2}, \quad (64)$$

where we have used the following formula:

$$\frac{\wp'}{\omega - \epsilon} = \text{Re} \frac{1}{(\omega - \epsilon + i0)^2} \quad (65)$$

for the derivative of the principal value, \wp' .

In other words, the full spectral function a has, in the extended quasi-particle approximation, as contrasted to the plain quasi-particle approximation, both pole and off-pole parts and it reads

$$a \approx \left(1 + \frac{\partial \sigma}{\partial \omega}\right) 2\pi\delta(\omega - \epsilon) + \text{Re} \frac{\gamma(\omega)}{(\omega - \epsilon + i0)^2}. \quad (66)$$

The plain quasi-particle approximation is extended by the off-pole part b of the spectral function.

$$a \approx 2\pi z\delta(\omega - \epsilon). \quad (67)$$

4.3.2. Sum rules for spectral function

Here, we show that contrary to the plain quasi-particle approximation, its extended form fulfills the sum rule (42).

Using the Kramers–Kronig relation

$$\sigma(\epsilon) = \sigma^\delta - \int \frac{d\omega}{2\pi} \gamma(\omega) \frac{\wp}{\omega - \epsilon}, \quad (68)$$

where σ^δ is the singular part of the self-energy, we find

$$\begin{aligned} \int \frac{d\omega}{2\pi} a &= \int \frac{d\omega}{2\pi} \left(1 + \frac{\partial \sigma}{\partial \omega}\right) 2\pi\delta(\omega - \epsilon) \\ &\quad + \int \frac{d\omega}{2\pi} \gamma \frac{\wp'}{\omega - \epsilon} \\ &= 1 + \frac{\partial \sigma}{\partial \epsilon} + \frac{\partial}{\partial \epsilon} \int \frac{d\omega}{2\pi} \gamma \frac{\wp}{\omega - \epsilon} = 1. \end{aligned} \quad (69)$$

We note that the extended quasi-particle approximation fulfills even the mean energy sum rule

$$\int \frac{d\omega}{2\pi} \omega a = \epsilon_k + \sigma^\delta(k, r, t), \quad (70)$$

which is not fulfilled by the plain quasi-particle approximation. For more details and for a comparison of the plain and extended quasi-particle approximations see the article by Kohler and Malfliet [34].

We can conclude that using the extended quasi-particle approximation, the first shortcoming of the Kadanoff–Baym approach is overcome.

4.3.3. Correlation functions in EQA

In analogy with the KB approximation (24) for $g^<$, for λ we use its near-to-equilibrium approximation

$$\lambda^<(\omega, k, r, t) = \phi(\omega, k, r, t)s(\omega, k, r, t), \quad (71)$$

and define the quasi-particle distribution $f(k, r, t)$ as the pole value of $\phi(\omega, k, r, t)$, i.e.

$$f(k, r, t) = \phi(\omega, k, r, t)_{\omega=\varepsilon}. \quad (72)$$

Using the approximation EQA for the spectral function s , see (61), we have

$$\lambda^< = f 2\pi z \delta(\omega - \varepsilon). \quad (73)$$

Similarly, using $f\gamma \approx \sigma^<$ and (64) we obtain

$$\xi^< = \sigma^< \frac{\phi'}{\omega - \varepsilon} = \text{Re} \frac{\sigma^<}{(\omega - \varepsilon + i0)^2}. \quad (74)$$

The full correlation function g in the limit of small scattering rates thus reads

$$\begin{aligned} g^< &\approx \lambda^< + \xi^< \\ &\approx f z 2\pi \delta(\omega - \varepsilon) + \text{Re} \frac{\sigma^<}{(\omega - \varepsilon + i0)^2}. \end{aligned} \quad (75)$$

The first term is just the quasi-particle approximation (the KB Ansatz) (34). The second term is an off-pole correction to the original KB ansatz. With reference to this additional term, this approximation of $g^<$ is called the extended quasi-particle approximation (EQA).

4.4. Boltzmann equation in EQA

To obtain the quasi-particle Boltzmann equation from (60) it now remains to follow the Kadanoff–Baym approach, using (73) in (60) (for details see [29]):

$$\frac{\partial f}{\partial t} + \frac{\partial \varepsilon}{\partial k} \frac{\partial f}{\partial r} - \frac{\partial \varepsilon}{\partial r} \frac{\partial f}{\partial k} = z \sigma_{\omega=\varepsilon}^< - f z \gamma_{\omega=\varepsilon}. \quad (76)$$

This kinetic equation has the same form as (37). There is, however, an essential difference in the

evaluation of the scattering integrals and observables from the distribution function f within the simple quasi-particle approximation in comparison with the EQA.

4.4.1. Scattering integrals in EQA

In the quasi-particle approximation, using the KB Ansatz, the self-energy in the scattering integrals of the final BE reads:

$$\sigma^<[g^<] = \sigma^<[f z 2\pi \delta(\omega - \varepsilon)] = \sigma^<[\lambda^<] = \sigma_{\lambda}^<(\omega). \quad (77)$$

Using the EQA (75), the self-energy in the scattering integrals reads:

$$\begin{aligned} \sigma^<(\omega) &= \sigma^<[\lambda^< + \xi^<] \\ &= \sigma^< \left[f z 2\pi \delta(\omega - \varepsilon) + \text{Re} \frac{\sigma_{\lambda}^<(\omega)}{(\omega - \varepsilon + i0)^2} \right], \end{aligned} \quad (78)$$

where we have used the fact that within the accuracy of the small γ expansion, the off-pole part $\lambda^<$ of $g^<$ can be approximated as

$$\xi^<(\omega) = \text{Re} \frac{\sigma_{\lambda}^<(\omega)}{(\omega - \varepsilon + i0)^2}. \quad (79)$$

Contrary to the standard KBA, this improved EQA makes possible a proper incorporation of two phonon processes in the scattering integrals; see discussions in [28,29].

The different recipe for the scattering integrals is not the only way in which the kinetic theory with included off-shell contributions within the EQA differs from the one based on the pole (simple quasi-particle) approximation. It also differs in the functional for evaluating the observables from the quasi-particle distribution function.

4.5. Observables

According to (19) in the Wigner representation we have

$$\rho = \int \frac{d\omega}{2\pi} g^< = \int \frac{d\omega}{2\pi} (\lambda^< + \xi^<). \quad (80)$$

Using the extended quasi-particle approximation (75) in this relation we will arrive at the reduced

density matrix, which is consistent within the small Γ expansion,

$$\rho = f z + \int \frac{d\omega}{2\pi} \frac{\wp}{\omega - \varepsilon} \frac{\partial \sigma_{\lambda}^{<}}{\partial \omega}, \quad (81)$$

where the off-pole contribution is integrated by parts. We note that within the quasi-particle approximation (KB Ansatz), only the first term is included.

There are two remarks which are worth mentioning:

1. As shown in Ref. [29] the above formula for observables provides backflows known from the Landau theory of Fermi liquids.

2. The above formula for ρ corrects the causality of the developed kinetic theory.

In other words, from the point of view of observables, the complete theory is causal, even if there is an acausal element in the kinetic equation for the quasi-particle distribution function related to the completed collisions.

4.6. Summary of the kinetic theory in EQA

We can overcome problems with the on-shell and off-shell character of processes in the derivation of the quasi-particle kinetic theory, if we do not strictly follow the original Kadanoff and Baym approach, but adopt the following scheme:

1. take the transport equation for $g^{<}$,
2. split this $g^{<}$ into its on-shell λ and off-shell ξ parts,
3. assign the quasi-classical limit of equations for λ and ξ ,
4. take the limit of small scattering rates (EQA).

The final kinetic theory consists of two constituents the quasi-particle kinetic equation and the functional which determines observables from the quasi-particle distribution function. The theory has the following properties:

1. Due to EQA, this kinetic theory is strictly valid only for weakly renormalized systems where $z = 1 + \frac{\partial \sigma}{\partial \omega}$,
2. Within this theory, the off-shell and on-shell contributions are treated consistently. Treating

consistently the on-shell and off-shell contributions, both on correlation and spectral functions levels, we obtain a kinetic theory, which is fully causal. At the same time, the idea of completed collisions, natural for the BE-like kinetic equations, is incorporated in the theory. Related acausality in the kinetic equation for the quasi-particle distribution function is corrected by the functional $\rho[f]$.

3. No linear gradients are neglected, and within this kinetic theory, there is a consistent separation of the explicit gradient terms on the left-hand side of the kinetic equation and the scattering integrals on the right-hand side.

5. Non-local kinetic theory and EQA

Till now, we have not taken into account the time and space non-localities of the real collisions. There is a related inner inconsistency already in the classical Boltzmann equation since, contrary to real scattering events, all collisions in this equation are described as local and instant ones. Thus, the BE is not thermodynamically consistent with virial corrections to the equation of state. This does not matter much for dilute gases, but non-localities of collisions of molecules of finite diameters have to be taken into account already in the case of moderately dense gases. Clausius was the first to introduce the description of non-local collisions to describe the thermodynamic properties of moderately dense gases [4,5]. He was followed by Enskog who derived generalization of the Boltzmann equation which takes into account finite diameters of colliding particles. This equation, called Enskog equation nowadays [3–5], is the well-known prototype of all kinetic equations with non-local scattering integrals. It provides the so-called virial corrections leading to equations of state of the non-ideal gas [4,5]; the BE generates only the equation of state of the ideal gas.

This section will deal with a natural question on how to incorporate virial corrections into the quasi-particle Boltzmann equation, i.e. how to derive a quantum version of the Enskog equation. As is known, virial corrections are related to the expansion of the pressure of equilibrium non-ideal

gases in terms of powers of the density. Already in 1937 Beth and Uhlenbeck showed that the concept of virial corrections can be generalized to quantum systems. They expressed the second virial correction via the on-shell derivatives of scattering phase shift with respect to the momentum of colliding particles [40]. As we will see in this section, the derivatives of scattering phase shifts also determine the non-local corrections to scattering integrals of quantum kinetic equations, which are thermodynamically consistent up to the second virial correction.

Many authors contributed to the effort to include virial corrections in quantum transport [41–57]. The main problem in obtaining a quasi-particle non-local kinetic theory was that very different methods were developed for treatment of virial and quasi-particle approximations. The virial corrections were discussed more from the point of view of chemical physics of dense gases, while quasi-particle corrections approaches rather used methods developed within the quantum Fermi liquid theory for condensed systems.

The important milestones achieved during derivation of a quantum non-local kinetic equation was the Waldman–Snider equation [42–45] and later on the works of Nacher, Tastevin and Laloe [48–50], and de Haan [51–53].

Snider was the first to derive a quantum kinetic equation with non-local corrections [42–44] generalizing the original Waldman equation [41]. The Waldman–Snider equation, however, was found to be inconsistent with the second-order virial corrections to the equation of state [46,47]. Laloe, Tastevin and Nacher [48–50] formulated a theory for non-degenerated quantum gases which contain, at the same time, quasi-particle renormalization and virial corrections consistent with the second-order virial corrections. This theory was independently confirmed by de Haan [51–53] who used a method different from the above authors (Balescu’s method for derivation of kinetic equations). The important aspect of this theory is that all non-local corrections are expressed via various derivatives of the scattering phase shift. This result is not surprising at all, when we look at information contained in the quantum mechanical description of collisions within the Landau theory of

quasi-particles. Differential cross sections are related to amplitudes of wave functions in the individual scattering channels. Quasi-particle wave function renormalization is provided by phase shifts in the non-dissipative zero angle scatterings. The only neglected information consists of phase shifts in dissipative scattering channels. We will show in the following text that these phase shifts will also determine the non-localities of scattering integrals of quasi-particle kinetic equations for a dense Fermi liquid derived from the NGF transport equations.

Within the NGF method, the non-local and non-instant contributions to the scattering integrals were introduced by Barwinkel for the first time in his kinetic theory of rare gases in his pioneering works [58]. His approach was, however, limited to low densities (he avoided medium effects on binary collisions). In addition, he used the quasi-particle approximation which has shortcoming that have been discussed in the previous sections. Especially, by neglecting the gradient term $[g, \sigma^<]$, treatment of linear gradients is not consistent. Later on, Bornath, Kraeft and Schlages developed a non-local kinetic theory using a variant of the EQA, which was, however, and not cover degenerated systems [35].

We will show here briefly that the kinetic theory reviewed in the last section also provides the basis for the consistent non-local kinetic theory for various, in general degenerate, quantum Fermi liquid systems. We address two rather general tasks of quantum statistical physics:

1. To create a kinetic theory consistent with thermodynamical behavior of observables.
2. To combine quasi-particle and virial corrections consistently in a quantum kinetic equation.

5.1. *Quasi-particle kinetic equation with collisional delay*

To demonstrate the main points of the non-local kinetic theory in the simplest possible way, we will start this section with the discussion of the theory for a system of non-interacting electrons scattered by resonant levels of neutral impurities which was developed in Refs. [59,60]. This means that instead

of full dynamics of binary collisions, we will take into account only electron-impurity scattering events which are described by momentum-independent self-energy.

To derive a non-local kinetic equation, in which both quasi-particle and virial corrections are included consistently, we apply the scheme for arriving at the quasi-particle kinetic theory discussed in the last section. We will start from the kinetic equation (76) derived within the EQA in Section 4.

It was shown in Ref. [60] that virial corrections consistent with the quasi-particle corrections can be obtained as linear gradient corrections to the scattering integrals, which come from the inner gradients of self-energy. These gradients, however, appear only if we deal with more complex self-energies than with the Born approximation. Therefore, in the second step, we use the averaged T -matrix approximation [60] to calculate linear gradients of the self-energy in scattering integrals of (76). By this step, we finally derive the following equation:

$$\begin{aligned} \frac{\partial f}{\partial t} + z \frac{k}{m} \frac{\partial f}{\partial r} - \frac{\partial U_{\text{eff}}}{\partial r} \frac{\partial f}{\partial k} \\ = -\frac{f}{\tau} + \frac{1}{\tau} \frac{2\pi^2}{k^2} \int \frac{dp}{(2\pi)^3} \delta(|p| - |k|) f(p, r, t) \\ - \frac{1}{\tau} \frac{2\pi^2}{k^2} \int \frac{dp}{(2\pi)^3} \delta(|p| - |k|) \Delta_t \frac{\partial}{\partial t} f(p, r, t). \end{aligned} \quad (82)$$

Due to the fixed positions of impurities, we do not have a full dynamics of binary collisions here. Correspondingly, we do not encounter any spatial non-localities given by momentum derivatives. The only non-zero linear gradient of the self-energy for resonant levels of impurities is its time derivative. We can rewrite the gradient-less and the time-gradient contribution to the scattering integral, in the approximation of the linear order of gradients, to obtain the following equation with a scattering integral non-local in time:

$$\begin{aligned} \frac{\partial f}{\partial t} + z \frac{k}{m} \frac{\partial f}{\partial r} - \frac{\partial U_{\text{eff}}}{\partial r} \frac{\partial f}{\partial k} \\ = -\frac{f}{\tau} + \frac{1}{\tau} \frac{2\pi^2}{k^2} \int \frac{dp}{(2\pi)^3} \\ \times \delta(|p| - |k|) f(p, r, t - \Delta_t). \end{aligned} \quad (83)$$

Here, the quasi-particle distribution f is a function of momentum k , coordinate r and time t . Lifetime τ , collision delay Δ_t and wave-function renormalization z are functions of momentum; the potential U_{eff} depends on coordinate and time. The lifetime τ is evaluated from the t -matrix of the system [60]

$$\frac{1}{\tau} = c(-2)\text{Im } t^{\text{R}}, \quad (84)$$

where c is the concentration of impurities.

5.1.1. Collision delay

The collision delay Δ_t is given by the energy derivative of the phase shift, or equivalently by the derivative of the t -matrix

$$\Delta_t = \text{Im} \frac{1}{t^{\text{R}}} \frac{\partial t^{\text{R}}}{\partial \omega} \Big|_{\omega=\epsilon_k} = \frac{\partial \phi}{\partial \omega} \Big|_{\omega=\epsilon_k}, \quad (85)$$

where $\phi = \text{Im} \ln t^{\text{R}}$ is the scattering phase shift. Formula (85) is just the delay time reflects already by Wigner [36–39]. This delay time reflects the attraction of an electron by an impurity and describes the inner dynamics of electron-impurity scattering.

5.1.2. Features of the non-local kinetic equation

Due to the collision time the scattering-integral is non-local in time. The time non-locality represents virial corrections, as will be seen later in this chapter from the expressions for observables. We can see that, in accordance with the works of Laloe, Tastevin and Nacher, non-locality is expressed by the derivative of t -matrix (phase shift). Since the self-energy of the model is momentum independent, the scattering integrals are local in space. The quasi-particle corrections are described by the wave-function renormalization z . Using NGF, we thus generated a non-local kinetic equation which corresponds to the intuitive picture of quasi-particle and virial corrections: the quasi-particle renormalization z influences the drift between collisions, so it enters the kinetic equation as a renormalization of velocity $v = z \frac{k}{m}$. In correspondence with the classical view of virial corrections and collisions, the virial corrections enter the scattering integral. Within the local approximations, when the collision delay is zero,

dynamics of the electron during the collision is neglected and the quasi-particle Boltzmann equation is obtained. We note that the kinetic equation (83) is Non-Markovian due to its non-local scattering integrals. Collisional delay is the reason why the initial and final states of collision occur at different times. There is, however, still an essential difference between the “true” Non-Markovian transport equations represented by the General Master Equations (GME) (see Paper I) and the kinetic equation (83). Contrary to the GME, there is no integration over the time to the past in this non-local kinetic equation.

5.2. Observables: quasi-particle and virial corrections

After having obtained the quasiparticle distribution f from the kinetic equation (83), we can calculate one particle observables from the functional between f and ρ , see the last section, formula (81).

5.2.1. Local density of electrons and Fermi momentum

The density of electrons is given by the integral of ρ over the momentum

$$n = \int \frac{dk}{(2\pi)^3} \rho. \quad (86)$$

Using formula (81) for ρ , we obtain, after several algebraic manipulations,

$$n = \int \frac{dk}{(2\pi)^3} f(k) \left(1 + \frac{\Delta_t}{\tau}\right), \quad (87)$$

The total (physical) density is thus the sum of two parts,

$$n = n_{\text{free}} + n_{\text{corr}}, \quad (88)$$

$$n_{\text{free}} = \int \frac{dk}{(2\pi)^3} f(k), \quad (89)$$

$$n_{\text{corr}} = \int \frac{dk}{(2\pi)^3} f(k) \frac{\Delta_t}{\tau}. \quad (90)$$

The free density n_{free} is the density of freely moving quasi-particles (electrons) between scatterings by

impurity levels, i.e. it has the meaning of the local density of quasi-particles. n_{corr} is called the correlated density since it describes the density correlated with impurities due to the finite collision delay Δ_t of electrons. It reflects the fact that due to impurity potentials which attract (repel) an electron from the vicinity of impurities, the density of free electrons is not equal to the physical density. Attraction of electrons by impurities reduces the density of free electrons by correlated density. When electrons are expelled from impurities the density increases.

We note that the total density (87) obtained from the reduced density-functional (81) is identical to the one obtained from the transport equation via the continuity equation. When we integrate kinetic equation (83) over momentum k , $\frac{\partial f}{\partial t}$ results in $\frac{\partial n_{\text{free}}}{\partial t}$, while the scattering integrals provide $\frac{\partial n_{\text{corr}}}{\partial t}$. The rest of the drift terms turn into the gradient of the density of the current. In other words, as for the total density, the approximative functional for the reduced density matrix (81) is consistent with the approximations in the kinetic equation (83).

The Fermi momentum is a parameter of the quasi-particle distribution f , so it is expressed (for the parabolic band) in terms of the free density as

$$k_F = \sqrt[3]{3\pi^2 n_{\text{free}}}. \quad (91)$$

For a low-density n , the ratio Δ_t/τ is only very weakly dependent on momentum k , so that we can approximate the relation between the total and free densities as

$$n = n_{\text{free}} \left(1 + \frac{\Delta_t}{\tau}\right), \quad (92)$$

which enables us to express the Fermi momentum in terms of the physical density as

$$k_F = \sqrt[3]{\frac{3\pi^2 n}{1 + \frac{\Delta_t}{\tau}}}. \quad (93)$$

5.2.2. Local density of current

A formula for the current is

$$j = \int \frac{dk}{(2\pi)^3} \frac{\partial \varepsilon}{\partial k} \rho = \int \frac{dk}{(2\pi)^3} \frac{k}{m} \rho. \quad (94)$$

When we substitute for ρ , we obtain

$$\begin{aligned} j &= \int \frac{dk}{(2\pi)^3} \frac{k}{m} z f \\ &+ \int \frac{dk}{(2\pi)^3} \frac{d\omega}{2\pi} \frac{k}{m} \operatorname{Re} \frac{\sigma^<(\omega)}{(\omega - \varepsilon_k + i0)^2} \\ &= \int \frac{dk}{(2\pi)^3} \frac{k}{m} z f. \end{aligned} \quad (95)$$

The second term is zero, because its integrand is an odd function of momentum k . We see that, contrary to the density and Fermi momentum, there are no explicit virial corrections to the current.

Calculating the density of current directly from the kinetic equation, we obtain the same expression (95) from the equation of continuity for the current. Again, the consistency of approximations used for the kinetic equation and the observable (current) is confirmed.

5.2.3. Local density of energy

Since we have the EQA for the correlation function, we can even obtain the local density of energy. The energy is not a single-particle observable, and has to be evaluated directly from the correlation function

$$E = \int \frac{d\omega}{2\pi} \frac{dk}{(2\pi)^3} \omega g^<(\omega, k). \quad (96)$$

As a result we obtain the local energy in terms of the collision delay

$$E = \int \frac{dk}{(2\pi)^3} \varepsilon_k f(k) \left(1 + \frac{A_I}{\tau} \right). \quad (97)$$

The thermodynamical consistency of the total energy conservation and correlated density is shown in Ref. [60].

5.2.4. DC conductivity

We will mention the DC conductivity as an example of an observable, for which neither the quasi-particle nor the virial correction plays an important role. In the relaxation time approximation, the above kinetic theory provides the follow-

ing formula for the DC conductivity:

$$\sigma_{dc} = \frac{e^2 k_F^3 \tau}{3\pi^2 m} z. \quad (98)$$

Using formula (93) for k_F in terms of the total density

$$\sigma_{DC} = \frac{e^2 n \tau}{m} \frac{z}{1 + \frac{A_I}{\tau}} \approx \frac{e^2 n \tau}{m}, \quad (99)$$

we see that virial and quasi-particle corrections mutually compensate.

5.2.5. Relation between quasi-particle and virial corrections: Derived Optical Theorem

We saw that virial and quasi-particle corrections play various roles in different observables. Some observables depend only on the quasi-particle correction, some on the virial correction and some on both. Here, we would like to point out that these corrections are not independent, since they are mutually related by the Derived Optical Theorem.

In the case of the model of electrons scattered by impurities in a semiconductor the Derived Optical Theorem reads

$$\frac{A_I}{\tau} = \frac{\partial \sigma}{\partial \omega} - c |t^R|^2 \operatorname{Re} \frac{\partial}{\partial \omega} \langle 0 | G_0^R | 0 \rangle, \quad (100)$$

where $\langle 0 | G_0^R | 0 \rangle$ is the matrix element of Green function in the host semiconductor crystal; for details, see Refs. [59,60].

From the above formula we can immediately see a relation between the quasi-particle and virial corrections. It is just necessary to take into account that in the observables virial corrections are represented by the expression $1 + \frac{A_I}{\tau}$ while quasi-particle corrections by $z = 1 + \frac{\partial \sigma}{\partial \omega}$.

The Derived Optical Theorem also explains why most of the quasi-classical kinetic equations have only local scattering integrals and do not contain any virial corrections: these equations have been mostly derived for a regime of a weak potential, that means in the Born approximation. For the case of scattering by impurities, the Born approximation gives $t^R \approx v$, i.e. $\sigma = cv^2 \langle 0 | G_0^R | 0 \rangle$, so that the first term cancels the second term of (100). As a result, the virial corrections are negligible.

The case of scattering of electrons by resonant levels of impurities is, however, far from being described by the Born approximation. In fact, as shown in Ref. [59] in this situation the first term of (100) is much larger than the second one, and the second term can be neglected. It means that in this transport regime virial and quasi-particle corrections are almost the same.

5.3. Non-local kinetic theory for binary collisions

Here, we will only briefly comment on the basic aspects of the non-local kinetic theory for dense Fermi systems in the case of full quantum dynamics of binary collisions as it was formulated in Ref. [61].

The method of deriving this non-local kinetic theory is the same as that discussed in the previous section: (1) Use the same precursor of the kinetic equation (76) derived within the Extended quasi-particle approximation. (2) Specify the self-energy for scattering integrals. Contrary to the previous section we now wish to describe full quantum dynamics of binary collision in the scattering integrals. To this end a many-body system is now described by the two-particle T -matrix in the Bethe–Goldstone approximation. (3) Perform (on the right-hand side of (76)) the gradient expansion of the self-energy up to linear gradient terms. This expansion provides, apart from the usual non-gradient term (the known local scattering integral), 19 gradient terms. All these terms can be recollected into contributions to the scattering integrals, non-local in space and time, by a procedure similar to the recasting of the gradient term in (82). Again, similar to the previous non-local in time kinetic equation (83), all these corrections are proportional to derivatives of the scattering phase shift which is given by the T -matrix. The symmetry of the scattering integrals and the correspondence of the derived kinetic equation to the Enskog equation of the classical physics are discussed in Ref. [62].

5.3.1. Features of the non-local kinetic theory

The non-local kinetic theory discussed consists of a non-local kinetic equation for the quasi-particle distribution function and a functional which con-

nects the distribution function with observables. The theory has all the characteristics of the quasi-particle kinetic theory: the Markovian quasi-particle Boltzmann equation of the Landau–Fermi liquid theory is recovered, when all virial corrections are neglected. Virial corrections to the local scattering integrals of the quasi-particle Boltzmann equation are expressed in terms of shifts in space and time that characterize the non-locality of the scattering integrals. The space shifts correspond to the finite-diameter corrections to collisions of hard spheres. The time shift is identified as the collision delay. All shifts are given by derivatives of the scattering phase shift in a binary collision. The non-local kinetic equation and virial corrections to thermodynamic observables (the density of particles, the density of energy and the stress tensor) are consistent up to the second virial coefficient. Apart from being causal and gauge invariant, the theory provides conservation laws for the density, energy and stress tensor [61].

5.3.2. Non-local kinetic theory and quasi-particles

The presented non-local kinetic theory also has thermodynamic consequences which are not in agreement with the strict formulation of the Landau theory of quasi-particles. This is related to the appearance of the correlated density in the non-local theory, which is given by the collisional delay [61]. This correlated density corresponds to the expression for the equilibrium density of dense quantum systems known from the original work of Beth and Uhlenbeck [40,65]

$$n = n_{\text{free}} + 2n_{\text{free}}^2 B(T, n), \quad (101)$$

where n_{free} is the number of free particles and the second term in (101) ($n_{\text{free}}^2 B(T, n)$ is the number of correlated pairs) plays the role of correlated density. Density-dependent second virial coefficient is expressed via the two-particle scattering phase shift. It was shown in Refs. [63–65] that in equilibrium the Extended quasi-particle Approximation provides the second-order virial corrections. The non-local kinetic equation and related observables discussed are consistently derived within the non-equilibrium version of the EQA. In this sense, the reviewed non-local kinetic

theory is consistent with the second-order virial corrections.

The existence of correlated density is in contradiction to the postulate of the Landau–Fermi liquid theory that the density of quasi-particles equals the total density of particles—the correlated density for scatterings by impurities; see formulas (88)–(90), for a more general case of binary collisions see Ref. [61]. This brings us to the question to which of the two quasi-particle concepts (the phenomenologic or the microscopic one) is innate to the non-local kinetic theory. Landau’s phenomenologic concept is based on the variation of thermodynamic quantities. The microscopic concept is related to the single-particle spectrum given within Green functions by the singularity of the spectral function of the system. Variational and spectral concepts of quasi-particles are equivalent close to the ground state of the Fermi liquid system. They, however, begin to differ if the excitation of the system increases. Dissipative processes, which freeze out for low temperatures, play an essential role in this difference. As shown in Ref. [66] the variational approach works properly only if collisions are treated within the instantaneous and elastic approximation. Local and instantaneous collisions have no effect on the thermodynamic properties and if they are sufficient for the description of the system, the variational approach is sufficient; both quasi-particle concepts provide the same densities. This, however, does not mean that both approaches are completely the same. Even in this situation, the quasi-particle energies determined within these two concepts differ by the so-called rearrangement energy, which describes the effect of the time-dependent Pauli blocking on the scattering phase shift. The situation becomes even more complicated if non-localities of collisions are important for the description of the non-equilibrium system. In this case, not only as the quasi-particle energies differ in these two conceptions but also the density of spectral quasi-particles differs from the density of the constituents particles by the correlated density resulting from the spectral approach to the quasi-particles. The spectral concept of quasi-particles is more suitable for highly non-equilibrium dense Fermi systems.

5.3.3. Summary

We discussed the non-local kinetic theory based on the Extended quasi-particle approximation and an advanced description of the inner dynamics of collisions by T -matrix approximation. First, we showed in more detail the common features of the theory for the simple case of the scattering of electrons at resonant levels of impurities in semiconductors. In this case, the inner dynamics of collisions was described only by the collision delay time given by the T -matrix. Second, we briefly dealt with full dynamics of binary collisions for the case of a dense Fermi liquid. Three-particle collisions were not taken into account, since they still have not been understood and so they are beyond the scope of the contemporary quantum kinetic theories, including the one presented here. On the other hand, the so-called in-medium many-body processes are included through the T -matrix.

In conclusion, the non-local quantum kinetic equation discussed, parallels the Enskog equation of the classical physics only from the point of view of non-localities of scattering integrals, while the static and dynamical correlations due to many-particle scatterings are not taken into account.

The non-local theory presented was applied for the physics of heavy ion collisions [67,68]. For the case of nuclear matter it is thoroughly discussed in Ref. [69].

6. Conclusions

In this paper, we reviewed kinetic theories as asymptotic theories derived from the NGF transport equations in the quasi-classical limit. All the discussed theories rely on the concept of quasi-particles and a possibility by generalizing the idea of the Fluctuation–Dissipation Theorem out of equilibrium. There are various possibilities on how to generalize the original non-equilibrium quasi-particle concept used by Kadanoff and Baym. Their Ansatz for the particle correlation function gives rise to the whole family of related constructions, all of them having an acausal structure and leading to quasi-particle kinetic equations. A special position among them holds the extended quasi-particle approximation, which permits to

derive the kinetic equation incorporating, at the same time, the quasi-particle drift and scattering integrals with non-local corrections. If non-local corrections are negligible, this equation turns into the Landau–Boltzmann equation of the Fermi liquid theory. The complete transport theory consists of the quasi-particle kinetic equation and of a complementing functional, permitting to calculate average values of observables, describing the true particles, from the quasi-particle distribution function. This theory, at least in the extended quasi-particle model, is physically consistent: the causality is restored, the theory is gauge invariant and it conserves the total densities of particles and energy.

Acknowledgements

This research was partially supported by the Grant Agencies of the Czech Republic and of the Academy of Sciences within the grant projects 202/04/0585 and A1010404, respectively. The research was carried out by V.S. within the Institutional Research Plan AV0Z10100521 and by A.K. within the Institutional Research Plan AVOZ10100520, both financed by the Academy of Sciences of the Czech Republic. The work of B.V. is a part of the research programs MSM 0021620834 and MSM 0021620845 financed by the Ministry of Education of the Czech Republic.

Long years of collaboration with Pavel Lipavský, who contributed essentially to much of the material and ideas covered, are gratefully acknowledged. We are also grateful to Klaus Morawetz for friendly scientific collaboration and many inspiring conversations. We also thank A. MacKinnon, M. Bonitz, R. Zimmermann, D. Kremp, H. Haug, A.-P. Jauho, and C. Caroli for illuminating discussions.

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